More on a Conjecture about Tricyclic Graphs with Maximal Energy*

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Abstract

The energy $\mathcal{E}(G)$ of a simple graph G is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. This concept was introduced by I. Gutman in 1977. Recently, Aouchiche et al. proposed a conjecture about tricyclic graphs: If G is a tricyclic graphs on n vertices with $n = 20$ or $n \geq 22$, then $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6,6})$ with equality if and only if $G \cong P_n^{6,6,6}$, where $P_n^{6,6,6}$ denotes the graph with $n \geq 20$ vertices obtained from three copies of C_6 and a path P_{n-18} by adding a single edge between each of two copies of C_6 to one endpoint of the path and a single edge from the third C_6 to the other endpoint of the P_{n-18}. Li et al. [X. Li, Y. Shi, M. Wei, J. Li, On a conjecture about tricyclic graphs with maximal energy, *MATCH Commun. Math. Comput. Chem.* 72(1)(2014), 183-214] proved that the conjecture is true for graphs in the graph class $\mathcal{G}(n; a, b, k)$, where $\mathcal{G}(n; a, b, k)$ denotes the set of all connected bipartite tricyclic graphs on $n \geq 20$ vertices with three vertex-disjoint cycles C_a, C_b and C_k, apart from 9 subclasses of such graphs. In this paper, we improve the above result and prove that apart from 7 smaller subclasses of such graphs the conjecture is true for graphs in the graph class $\mathcal{G}(n; a, b, k)$.

1 Introduction

The energy $\mathcal{E}(G)$ of a simple graph G is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. This concept was introduced [8] by Gutman in 1977. For details about the graph energy, we refer the reader to two surveys [9,10] and the book [28]. A lot of results have been obtained on the minimal and maximal energies in some given classes of graphs, such as trees, unicyclic graphs, bycyclic graphs, etc.; see [1,2,5,7,13–27,30–33].

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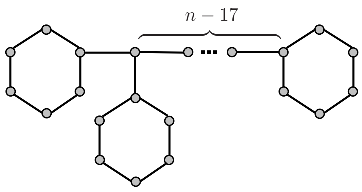
The problem of finding the tricyclic graphs maximizing the energy remains open. Gutman and Vidović [12] listed some tricyclic molecular graphs that might have maximal energy for $n \leq 20$. Very recently, experiments using AutoGraphiX led the authors of [3] to conjecture the structure of tricyclic graphs that presumably maximize energy for $n = 6, \dots, 21$. For $n \geq 22$, Aouchiche et al. [3] proposed a general conjecture obtained with AutoGraphiX. First, let $P_n^{6,6,6}$ (see Figure 3) denote the graph on $n \geq 20$ obtained from three copies of C_6 and a path P_{n-18} by adding a single edge between each of two copies of C_6 to one endpoint of the path and a single edge from the third C_6 to the other endpoint of the P_{n-18}.

Conjecture 1.1 [3] *Let G be a tricyclic graphs on n vertices with $n = 20$ or $n \geq 22$. Then $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6,6})$ with equality if and only if $G \cong P_n^{6,6,6}$.*



$P_n^{6,6,6}$

Figure 1: Tricyclic graph $P_n^{6,6,6}$.

Let $\mathcal{G}(n; a, b, k)$ denote the set of all connected bipartite tricyclic graphs on n vertices with three disjoint cycles C_a, C_b and C_k, where $n \geq 20$. In this paper, we try to prove that the conjecture is true for graphs in the class $\mathcal{G}(n; a, b, k)$, but as a consequence we can only show that this is true for most of the graphs in the class except for 9 families of such graphs. From the definition of $\mathcal{G}(n; a, b, k)$, we know that a, b and k are all even. We will divide $\mathcal{G}(n; a, b, k)$ into two categories $\mathcal{G}_I(n; a, b, k; \ell_1, \ell_2; \ell_c)$ and $\mathcal{G}_{II}(n; a, b, k; \ell_1, \ell_2, \ell_3)$ in the following. We say that H is the *central structure* of G if G can be viewed as the graph obtained from H by planting some trees on it. Denote by $\mathcal{H}_I(n; a, b, k; \ell_1, \ell_2; \ell_c)$ and $\mathcal{H}_{II}(n; a, b, k; \ell_1, \ell_2, \ell_3)$ the central structures of $\mathcal{G}_I(n; a, b, k; \ell_1, \ell_2; \ell_c)$ and $\mathcal{G}_{II}(n; a, b, k; \ell_1, \ell_2, \ell_3)$, respectively.

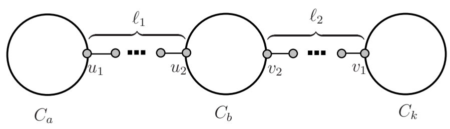


Figure 2: $\mathcal{H}_I(n; a, b, k; \ell_1, \ell_2; \ell_c)$.

The graph class $\mathcal{H}_I(n; a, b, k; \ell_1, \ell_2; \ell_c)$ (see Figure 2) is the set of all the elements of $\mathcal{G}(n; a, b, k)$ in which C_a and C_b are joined by a path $P_1 = u_1 \cdots u_2$ ($u_2 \in V(C_b)$) with ℓ_1 vertices, C_k and C_b are joined by a path $P_2 = v_1 \cdots v_2$ ($v_2 \in V(C_b)$) with ℓ_2 vertices. In addition, the smaller part $u_2 \cdots v_2$ of C_b has ℓ_c vertices. When $u_2 = v_2$, we have $\ell_c = 1$.

The graph class $\mathcal{H}_{II}(n; a, b, k; \ell_1, \ell_2, \ell_3)$ (see Figure 3) is also a subset of $\mathcal{G}(n; a, b, k)$. For any $H \in \mathcal{H}_{II}(n; a, b, k; \ell_1, \ell_2, \ell_3)$, h has a center vertex v, C_a, C_b and C_k are joined to v by paths $P_1 = u_1 \cdots v$ $(u_1 \in V(C_a))$, $P_2 = u_2 \cdots v$ $(u_2 \in V(C_b))$, $P_3 = u_3 \cdots v$ $(u_3 \in V(C_k))$, respectively. The number of vertices of P_1, P_2 and P_3 are ℓ_1, ℓ_2 and ℓ_3, respectively.

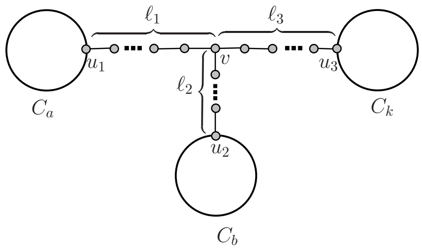


Figure 3: $\mathcal{H}_{II}(n; a, b, k; \ell_1, \ell_2, \ell_3)$.

It is clear that

$$\mathcal{G}(n; a, b, k) = \mathcal{G}_I(n; a, b, k; \ell_1, \ell_2; \ell_c) \cup \ \mathcal{G}_{II}(n; a, b, k; \ell'_1, \ell'_2, \ell'_3).$$

Now we introduce two special graph classes $\mathcal{H}_1^*$ and $\mathcal{H}_2^*$ as follows.

The graph class $\mathcal{H}_1^*$ consists of graphs H with the following four different possible forms:
(i) $H \in \mathcal{H}_I(n; a, 4, k; \ell_1, \ell_2; 2)$, where $a \geq 8$, $k \geq 8$, $2 \leq \ell_1 \leq 3$, $2 \leq \ell_2 \leq 3$.
(ii) $H \in \mathcal{H}_I(n; a, b, k; \ell_1, \ell_2; 2)$, where $a \geq 8$, $b \geq 6$, $k \geq 8$, $2 \leq \ell_1 \leq 3$, $2 \leq \ell_2 \leq 3$ and $\ell_1 = \ell_2 = 3$ is not allowed.
(iii) $H \in \mathcal{H}_I(n; 4, b, k; \ell_1, \ell_2; 2)$, where $b \geq 6$, $k \geq 6$, $2 \leq \ell_1 \leq 3$ and $2 \leq \ell_2 \leq 3$.
(iv) $H \in \mathcal{H}_I(n; a, b, 4; \ell_1, \ell_2; 2)$, where $2 \leq \ell_2 \leq 3$.
Whereas $\mathcal{H}_2^*$ consists of graphs H with the following five different possible forms:
(i) $H \in \mathcal{H}_{II}(n; a, b, k; 2, \ell_2, \ell_3)$, where $a \geq 8$.
(ii) $H \in \mathcal{H}_{II}(n; a, b, k; 3, 3, 3)$, where $a \geq k \geq b \geq 8$.
(iii) $H \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 3, \ell_3)$.
(iv) $H \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 2, \ell_3)$.
(v) $H \in \mathcal{H}_{II}(n; a, 4, k; 3, 4, 3)$, where $a \geq k \geq 6$.

In [29], the authors tried to find the graphs with maximal energy among the two categories of $\mathcal{G}(n; a, b, k)$: $\mathcal{G}_I(n; a, b, k; \ell_1, \ell_2; \ell_c)$ and $\mathcal{G}_{II}(n; a, b, k; \ell_1, \ell_2, \ell_3)$, respectively. Apart from two classes $\mathcal{H}_1^*$ and $\mathcal{H}_2^*$, they obtained that $P_n^{6,6,6} = \mathcal{H}_{II}(n; 6, 6, 6; n-17, 2, 2)$ has the maximal energy among all graphs in $\mathcal{G}(n; a, b, k)$. Their main result is stated as follows, which gives support to Conjecture 1.1.

Theorem 1.2 [29] *For any tricyclic bipartite graph* $G \in \mathcal{G}(n; a, b, k) \setminus (\mathcal{H}_1^* \cup \mathcal{H}_2^*)$, $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6,6})$ *and the equality holds if and only if* $G \cong P_n^{6,6,6}$.

In this paper, we try to improve the above result. Let us now introduce two graph classes $\mathcal{H}_1^{**}$ and $\mathcal{H}_2^{**}$. The graph class $\mathcal{H}_1^{**}$ consists of graphs H with the following three different possible forms:
(i) $H \in \mathcal{H}_I(n; a, 4, k; \ell_1, \ell_2; 2)$, where $a \geq 8$, $k \geq 8$, $2 \leq \ell_1 \leq 3$, $2 \leq \ell_2 \leq 3$.
(ii) $H \in \mathcal{H}_I(n; a, b, k; \ell_1, \ell_2; 2)$, where $a \geq 8$, $b \geq 6$, $k \geq 8$, $2 \leq \ell_1 \leq 3$, $2 \leq \ell_2 \leq 3$ and $\ell_1 = \ell_2 = 3$ is not allowed.
(iii) $H \in \mathcal{H}_I(n; a, b, 4; \ell_1, \ell_2; 2)$, where $2 \leq \ell_2 \leq 3$.
Whereas $\mathcal{H}_2^{**}$ consists of graphs H with the following four different possible forms:
(i) $H \in \mathcal{H}_{II}(n; a, b, k; 2, \ell_2, \ell_3) \cup \mathcal{H}_{II}(n; a, 6, 6; 2, \ell_2', \ell_3')$, where $a \geq 8$, $\ell_3' \geq 8$, and $\ell_1 = 2$ or $\ell_3 = 2$ or $6 \leq a + \ell_1 \leq 7$ or $6 \leq k + \ell_3 \leq 13$.
(ii) $H \in \mathcal{H}_{II}(n; a, b, k; 3, 3, 3)$, where $a \geq k \geq b \geq 8$, and $a \equiv 0 \ (mod\ 4)$ or $k \equiv 0 \ (mod\ 4)$.
(iii) $H \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 3, \ell_3)$, where $\ell_1 = 2$ or $\ell_3 = 2$ or $6 \leq a + \ell_1 \leq 7$ or $6 \leq k + \ell_3 \leq 13$.
(iv) $H \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 2, \ell_3) \cup \mathcal{H}_{II}(n; 6, 4, 6; 2, 2, \ell)$, where $\ell \geq 8$, and $\ell_1 = 2$ or $\ell_3 = 2$ or $6 \leq a + \ell_1 \leq 7$ or $6 \leq k + \ell_3 \leq 13$.

We obtain the following theorem, whose proof will be given in Section 3.

Theorem 1.3 *For any tricyclic bipartite graph $G \in \mathcal{G}(n; a, b, k) \setminus (\mathcal{H}_1^{**} \cup \mathcal{H}_2^{**})$, $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6,6})$ and the equality holds if and only if $G \cong P_n^{6,6,6}$.*

2 Preliminaries

In the sequel, let P_n, C_n, P_n^a and $P_n^{a,b}$ be a path, cycle, the graph obtained by connecting a vertex of the cycle C_a with a terminal vertex of the path P_{n-a}, the graph obtained from cycles C_a and C_b by joining a path of order $n - a - b + 2$, respectively. We refer to [4] for graph theoretical notation and terminology not described here.

The following are some elementary results on the characteristic polynomial of graphs and graph energy, which will be used later.

Lemma 2.1 [6] *Let uv be an edge of a graph G. Then*

$$\phi(G, \lambda) = \phi(G - uv, \lambda) - \phi(G - u - v, \lambda) - 2 \sum_{C \in \varphi(uv)} \phi(G - C, \lambda),$$

where $\phi(G, \lambda)$ denotes the characteristic polynomial of G, and $\varphi(uv)$ is the set of cycles of G containing uv. In particular, if uv is a pendant edge of G with the pendant vertex v, then

$$\phi(G, \lambda) = \lambda \phi(G - v, \lambda) - \phi(G - u - v, \lambda).$$

Lemma 2.2 [29] *Let uv be an edge of a bipartite tricyclic graph G which contains three vertex-disjoint cycles. Then*

$$b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v) + 2\sum_{C_l\in\varphi(uv)} (-1)^{1+\frac{l}{2}} b_{2i-l}(G-C_l),$$

where $\varphi(uv)$ is the set of cycles of G containing uv. In particular, if uv is a pendant edge of G with the pendant vertex v, then

$$b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v).$$

It is well-known [6] that if G is a bipartite graph, then the characteristic polynomial of G has the following form

$$\phi(G,\lambda) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i b_{2i} \lambda^{n-2i},$$

where $b_{2i} \geq 0$ for all $i = 1, \cdots, \lfloor \frac{n}{2} \rfloor$. For two bipartite graphs G_1 and G_2, Gutman and Polansky in [11] defined a quasi-order $G_1 \preceq G_2$ or $G_2 \succeq G_1$ if $b_{2i}(G_1) \leq b_{2i}(G_2)$ hold for all $i = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$; moreover, $G_1 \prec G_2$ or $G_2 \succ G_1$ if $b_{2i}(G_1) < b_{2i}(G_2)$ holds for some i. The above quasi-order implies the following quasi-order relation on graph energy

$$G_1 \preceq G_2 \Rightarrow \mathcal{E}(G_1) \leq \mathcal{E}(G_2), \quad G_1 \prec G_2 \Rightarrow \mathcal{E}(G_1) < \mathcal{E}(G_2).$$

From Sachs Theorem [6], we can obtain the following properties for bipartite graphs.

Lemma 2.3 [6] (1) *If G_1 and G_2 are both bipartite graphs, then $b_{2k}(G_1 \cup G_2) = \sum_{i=0}^{k} b_{2i}(G_1) \cdot b_{2k-2i}(G_2)$.*
(2) *If G_0, G_1, G_2 are all bipartite and $G_1 \preceq G_2$, since $b_{2i}(G_0) \geq 0$ and $b_{2i}(G_1) \geq b_{2i}(G_2)$ for all positive integer i, we have $G_0 \cup G_1 \preceq G_0 \cup G_2$. Moreover, for bipartite graphs G_i, G_i', $i = 1, 2$, if G_i has the same order as G_i' and $G_i \preceq G_i'$, then $G_1 \cup G_2 \preceq G_1' \cup G_2'$.*

Lemma 2.4 [11] *Let $n = 4k, 4k+1, 4k+2$ or $4k+3$. Then*

$$\begin{aligned} P_n &\succ P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \cdots \succ P_{2k} \cup P_{n-2k} \succ P_{2k+1} \cup P_{n-2k-1} \\ &\succ P_{2k-1} \cup P_{n-2k+1} \succ \cdots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}. \end{aligned}$$

3 Proof of Theorem 1.3

We are now in a position to prove our main result.

3.1 For (v) of the graph class $\mathcal{H}_2^*$

In [29], the authors obtained the following lemma.

Lemma 3.1 [29] *For any graph $H \in \mathcal{H}_{II}(n; 6, 6, 6; \ell_1, 2, \ell_3) \setminus P_n^{6,6,6}$, $H \prec P_n^{6,6,6}$.*

Proposition 3.2 *For any graph $H_1 \in \mathcal{H}_{II}(n; a, 4, k; 3, 4, 3)$ where $a \geq k \geq 6$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; 6, 6, 6; \ell_1, 2, \ell_3)$ such that $H_1 \preceq H_2$.*

Proof. Fix parameter n. For any $H_1 \in \mathcal{H}_{II}(n; a, 4, k; 3, 4, 3)$, we choose a graph $H_2 \in \mathcal{H}_{II}(n; 6, 6, 6; \ell_1, 2, \ell_3)$ such that $\ell_1 = a - 3$ and $\ell_3 = k - 3$ (see Figure 4). It suffices to show that $H_1 \preceq H_2$. From Lemma 2.2, we have

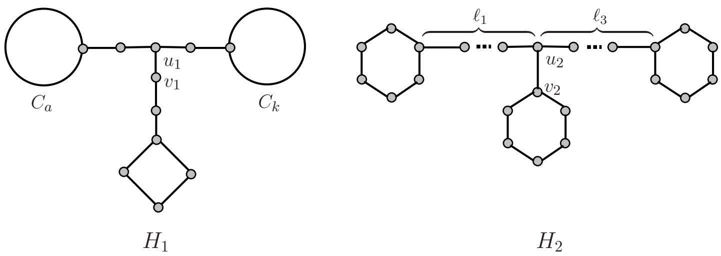


Figure 4: Graphs for Proposition 3.2

$$
\begin{aligned}
b_{2i}(H_1) &= b_{2i}(H_1 - u_1v_1) + b_{2i-2}(H_1 - u_1 - v_1) \\
&= b_{2i}(P_{a+k+3}^{a,k} \cup P_6^4) + b_{2i-2}(P_{a+1}^a \cup P_{k+1}^k \cup P_5^4) \\
b_{2i}(H_2) &= b_{2i}(H_2 - u_2v_2) + b_{2i-2}(H_2 - u_2 - v_2) \\
&= b_{2i}(P_{\ell_1+\ell_3+9}^{6,6} \cup C_6) + b_{2i-2}(P_{\ell_1+4}^6 \cup P_{\ell_3+4}^6 \cup P_5)
\end{aligned}
$$

Since $\phi(P_6^4; \lambda) = \lambda^6 - 6\lambda^4 + 6\lambda^2$ and $\phi(C_6; \lambda) = \lambda^6 - 6\lambda^4 + 9\lambda^2 - 4$, it follows that $P_6^4 \prec C_6$. Similarly, $\phi(P_5^4; \lambda) = \lambda^5 - 3\lambda^3 + 2\lambda$ and $\phi(P_5; \lambda) = \lambda^5 - 4\lambda^3 + 3\lambda$ yields $P_5^4 \prec P_5$. Because $\ell_1 = a - 3$ and $\ell_3 = k - 3$, we have $a + k + 3 = \ell_1 + \ell_3 + 9$, $a + 1 = \ell_1 + 4$ and $k + 1 = \ell_3 + 4$. Since $P_{a+1}^a \preceq P_{\ell_1+4}^6$, $P_{k+1}^k \preceq P_{\ell_3+4}^6$ and $P_{a+k+3}^{a,k} \preceq P_{\ell_1+\ell_3+9}^{6,6}$, we have $H_1 \preceq H_2$ by Lemma 2.3. ∎

Remark 1. Proposition 3.2 indicates that the energy of any graph in $\mathcal{H}_{II}(n; a, 4, k; 3, 4, 3)$ is not larger than the energy of a graph in $\mathcal{H}_{II}(n; 6, 6, 6; \ell_1, 2, \ell_3)$ with $\ell_1 = a - 3$ and $\ell_3 = k - 3$. From Lemma 3.1, $H \prec P_n^{6,6,6}$ for any graph $H \in \mathcal{H}_{II}(n; 6, 6, 6; \ell_1, 2, \ell_3)$ satisfying $H \neq P_n^{6,6,6}$. So we exclude the possibility of any graph in (v) of the graph class $\mathcal{H}_2^*$ posses maximal energy among all the tricyclic graphs and hence (v) of the graph class $\mathcal{H}_2^*$ can be deleted in Theorem 1.3.

3.2 For (iii) of the graph class $\mathcal{H}_2^*$

Now we focus our attention on (iii) of the graph class $\mathcal{H}_2^*$. For $H \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 3, \ell_3)$, one can see that there is no restrictive conditions on the parameters a, k, ℓ_1, ℓ_3. In this section, we shall show that if $\ell_1 \geq 3$, $\ell_3 \geq 3$, $a + \ell_1 \geq 8$ and $k + \ell_3 \geq 14$ then $H \prec P_n^{6,6,6}$ for any $H \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 3, \ell_3)$. Therefore, we narrow the scope of this graph class by putting extra conditions $\ell_1 = 2$ or $\ell_3 = 2$ or $5 \leq a + \ell_1 \leq 7$ or $5 \leq k + \ell_3 \leq 13$, which is stated as (iii) of the graph class $\mathcal{H}_2^{**}$ in Theorem 1.3.

Lemma 3.3 *For any graph $H_1 \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 3, \ell_3)$ where $\ell_1 \geq 3$, $\ell_3 \geq 3$, $a + \ell_1 \geq 8$ and $k + \ell_3 \geq 14$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; 6, 4, 6; \ell_1', 3, \ell_3')$ such that $H_1 \preceq H_2$.*

Proof. Fix parameter n. For any $H_1 \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 3, \ell_3)$, we choose a graph $H_2 \in \mathcal{H}_{II}(n; 6, 4, 6; \ell_1', 3, \ell_3')$ where $\ell_1' = a + \ell_1 - 6$ and $\ell_3' = k + \ell_3 - 6$ (see Figure 5). Since $k + \ell_3 \geq 14$, it follows that $\ell_3' \geq 8$. So we only need to show that $H_1 \preceq H_2$. From Lemma 2.2, we have

$$\begin{aligned}
b_{2i}(H_1) &= b_{2i}(H_1 - u_1v_1) + b_{2i-2}(H_1 - u_1 - v_1) \\
&= b_{2i}(P_{n-5}^{a,k} \cup P_5^4) + b_{2i-2}(P_{a+\ell_1-2}^{a} \cup P_{k+\ell_3-2}^{k} \cup C_4) \\
b_{2i}(H_2) &= b_{2i}(H_2 - u_2v_2) + b_{2i-2}(H_2 - u_2 - v_2) \\
&= b_{2i}(P_{n-5}^{6,6} \cup P_5^4) + b_{2i-2}(P_{a+\ell_1-2}^{6} \cup P_{k+\ell_3-2}^{6} \cup C_4)
\end{aligned}$$

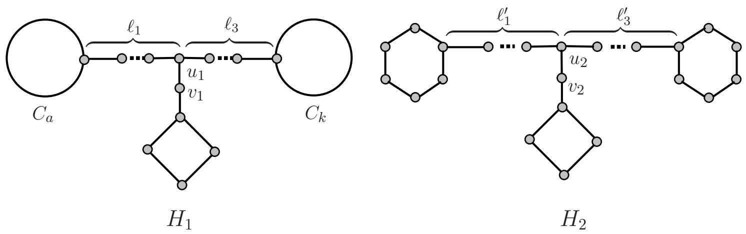


Figure 5: Graphs for Lemma 3.3.

Since $P_{n-5}^{a,k} \preceq P_{n-5}^{6,6}$, $P_{a+\ell_1-2}^{a} \preceq P_{a+\ell_1-2}^{6}$ and $P_{k+\ell_3-2}^{k} \preceq P_{k+\ell_3-2}^{6}$, it follows from Lemma 2.3 that $H_1 \preceq H_2$, as desired. ∎

Lemma 3.4 *For any graph $H_1 \in \mathcal{H}_{II}(n; 6, 4, 6; \ell_1, 3, \ell_3)$ where $\ell_3 \geq 8$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; 6, 4, 6; 2, 3, \ell)$ such that $H_1 \prec H_2$.*

Proof. Fix parameter n. For any $H_1 \in \mathcal{H}_{II}(n; 6, 4, 6; \ell_1, 3, \ell_3)$, we select a graph $H_2 \in \mathcal{H}_{II}(n; 6, 4, 6; 2, 3, \ell)$ where $\ell = \ell_1 + \ell_3 - 2$ (see Figure 6). Since $\ell_1 \geq 2$ and $\ell_3 \geq 8$, it follows that $\ell \geq 8$. We only need to show that $H_1 \prec H_2$. Using Lemma 2.2, we have

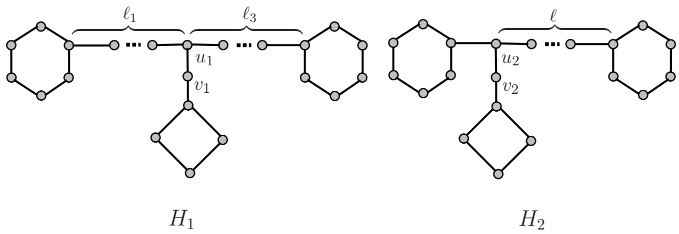


Figure 6: Graphs for Lemma 3.4.

$$\begin{aligned}
b_{2i}(H_1) &= b_{2i}(H_1 - u_1v_1) + b_{2i-2}(H_1 - u_1 - v_1) \\
&= b_{2i}(P_{n-5}^{6,6} \cup P_5^4) + b_{2i-2}(P_{\ell_1+4}^6 \cup P_{\ell_3+4}^6 \cup C_4)
\end{aligned}$$

$$\begin{aligned}
b_{2i}(H_2) &= b_{2i}(H_2 - u_2v_2) + b_{2i-2}(H_2 - u_2 - v_2) \\
&= b_{2i}(P_{n-5}^{6,6} \cup P_5^4) + b_{2i-2}(C_6 \cup P_{\ell+4}^6 \cup C_4)
\end{aligned}$$

From Lemma 2.3, we need to prove $P_{\ell_1+4}^6 \cup P_{\ell_3+4}^6 \prec C_6 \cup P_{\ell+4}^6$. Clearly, we have

$$\begin{aligned}
b_{2j}(P_{\ell_1+4}^6 \cup P_{\ell_3+4}^6) &= b_{2j}(C_6 \cup P_{\ell_1-2} \cup P_{\ell_3+4}^6) + b_{2j-2}(P_5 \cup P_{\ell_1-3} \cup P_{\ell_3+4}^6) \\
b_{2j}(C_6 \cup P_{\ell+4}^6) &= b_{2j}(C_6 \cup P_{\ell_1-2} \cup P_{\ell_3+4}^6) + b_{2j-2}(C_6 \cup P_{\ell_1-3} \cup P_{\ell_3+3}^6)
\end{aligned}$$

By Lemma 2.3, it suffices to show $P_5 \cup P_{\ell_3+4}^6 \prec C_6 \cup P_{\ell_3+3}^6$. We can easily obtain the following equalities.

$$\begin{aligned}
b_{2r}(P_5 \cup P_{\ell_3+4}^6) &= b_{2r}(P_5 \cup P_{\ell_3+3}^6 \cup P_1) + b_{2r-2}(P_5 \cup P_{\ell_3+2}^6) \\
&= b_{2r}(P_5 \cup P_{\ell_3+3}^6 \cup P_1) + b_{2r-2}(P_4 \cup P_1 \cup P_{\ell_3+2}^6) + b_{2r-4}(P_3 \cup P_{\ell_3+2}^6) \\
&= b_{2r}(P_5 \cup P_{\ell_3+3}^6 \cup P_1) + b_{2r-2}(P_4 \cup P_1 \cup P_{\ell_3+2}^6) + b_{2r-4}(P_3 \cup P_{\ell_3+1}^6 \cup P_1) \\
&\quad + b_{2r-6}(P_3 \cup P_{\ell_3}^6) \\
&= b_{2r}(P_5 \cup P_{\ell_3+3}^6 \cup P_1) + b_{2r-2}(P_4 \cup P_1 \cup P_{\ell_3+2}^6) + b_{2r-4}(P_3 \cup P_{\ell_3+1}^6 \cup P_1) \\
&\quad + b_{2r-6}(P_2 \cup P_1 \cup P_{\ell_3}^6) + b_{2r-8}(P_1 \cup P_{\ell_3}^6) \\
&= b_{2r}(P_5 \cup P_{\ell_3+3}^6 \cup P_1) + b_{2r-2}(P_4 \cup P_1 \cup P_{\ell_3+2}^6) + b_{2r-4}(P_3 \cup P_{\ell_3+1}^6 \cup P_1) \\
&\quad + b_{2r-6}(P_2 \cup P_1 \cup P_{\ell_3}^6) + b_{2r-8}(P_1 \cup P_{\ell_3-1}^6 \cup P_1) + b_{2r-10}(P_1 \cup P_{\ell_3-2}^6)
\end{aligned}$$

$$\begin{aligned}
b_{2r}(C_6 \cup P_{\ell_3+3}^6) &= b_{2r}(P_6 \cup P_{\ell_3+3}^6) + b_{2r-2}(P_4 \cup P_{\ell_3+3}^6) + 2b_{2r-6}(P_{\ell_3+3}^6) \\
&= b_{2r}(P_6 \cup P_{\ell_3+3}^6) + b_{2r-2}(P_4 \cup P_1 \cup P_{\ell_3+2}^6) + b_{2r-4}(P_4 \cup P_{\ell_3+1}^6) \\
&\quad + 2b_{2r-6}(P_{\ell_3+3}^6) \\
&= b_{2r}(P_6 \cup P_{\ell_3+3}^6) + b_{2r-2}(P_4 \cup P_1 \cup P_{\ell_3+2}^6) + b_{2r-4}(P_3 \cup P_1 \cup P_{\ell_3+1}^6) \\
&\quad + b_{2r-6}(P_2 \cup P_{\ell_3+1}^6) + 2b_{2r-6}(P_{\ell_3+3}^6) \\
&= b_{2r}(P_6 \cup P_{\ell_3+3}^6) + b_{2r-2}(P_4 \cup P_1 \cup P_{\ell_3+2}^6) + b_{2r-4}(P_3 \cup P_1 \cup P_{\ell_3+1}^6)
\end{aligned}$$

$$
\begin{aligned}
&+b_{2r-6}(P_2 \cup P_1 \cup P^6_{\ell_3}) + b_{2r-8}(P_2 \cup P^6_{\ell_3-1}) + 2b_{2r-6}(P^6_{\ell_3+3}) \\
= \; & b_{2r}(P_6 \cup P^6_{\ell_3+3}) + b_{2r-2}(P_4 \cup P_1 \cup P^6_{\ell_3+2}) + b_{2r-4}(P_3 \cup P_1 \cup P^6_{\ell_3+1}) \\
&+b_{2r-6}(P_2 \cup P_1 \cup P^6_{\ell_3}) + b_{2r-8}(P_1 \cup P_1 \cup P^6_{\ell_3-1}) + b_{2r-10}(P^6_{\ell_3-1}) \\
&+2b_{2r-6}(P^6_{\ell_3+3}) \\
= \; & b_{2r}(P_6 \cup P^6_{\ell_3+3}) + b_{2r-2}(P_4 \cup P_1 \cup P^6_{\ell_3+2}) + b_{2r-4}(P_3 \cup P_1 \cup P^6_{\ell_3+1}) \\
&+b_{2r-6}(P_2 \cup P_1 \cup P^6_{\ell_3}) + b_{2r-8}(P_1 \cup P_1 \cup P^6_{\ell_3-1}) + b_{2r-10}(P^6_{\ell_3-2} \cup P_1) \\
&+b_{2r-12}(P^6_{\ell_3-3}) + 2b_{2r-6}(P^6_{\ell_3+3})
\end{aligned}
$$

One can easily see that $P_5 \cup P^6_{\ell_3+4} \prec C_6 \cup P^6_{\ell_3+3}$, which implies $H_1 \prec H_2$. The result follows. ∎

Lemma 3.5 *For any graph $H_1 \in \mathcal{H}_{II}(n; 6, 4, 6; 2, 3, \ell)$ where $\ell \geq 8$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; 6, 6, 6; 2, 2, \ell')$ such that $H_1 \prec H_2$.*

Proof. Fix parameter n. For any $H_1 \in \mathcal{H}_{II}(n; 6, 4, 6; 2, 3, \ell)$, we choose a graph $H_2 \in \mathcal{H}_{II}(n; 6, 6, 6; 2, 2, \ell')$ where $\ell' = \ell - 1$ (see Figure 7). It suffices to show that $H_1 \prec H_2$. From

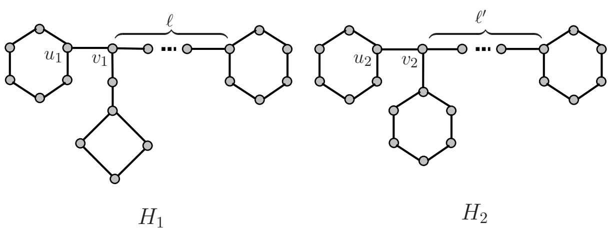


Figure 7: Graphs for Lemma 3.5.

Lemma 2.2, we have

$$
\begin{aligned}
b_{2i}(H_1) &= b_{2i}(H_1 - u_1v_1) + b_{2i-2}(H_1 - u_1 - v_1) \\
&= b_{2i}(P^{6,4}_{n-6} \cup C_6) + b_{2i-2}(P_5 \cup P^6_{\ell+4} \cup P^4_5) \\
b_{2i}(H_2) &= b_{2i}(H_2 - u_2v_2) + b_{2i-2}(H_2 - u_2 - v_2) \\
&= b_{2i}(P^{6,6}_{n-6} \cup C_6) + b_{2i-2}(P_5 \cup P^6_{\ell+3} \cup C_6)
\end{aligned}
$$

From Lemma 2.3, we need to prove $P^6_{\ell+4} \cup P^4_5 \prec P^6_{\ell+3} \cup C_6$. Clearly, we have

$$
b_{2j}(P^6_{\ell+4} \cup P^4_5) = b_{2j}(P^6_{\ell+4} \cup P_5) + b_{2j-2}(P^6_{\ell+4} \cup P_2 \cup P_1)
$$

where

$$
\begin{aligned}
b_{2j}(P^6_{\ell+4} \cup P_5) &= b_{2j}(P^6_{\ell+3} \cup P_5 \cup P_1) + b_{2j-2}(P^6_{\ell+2} \cup P_5) \\
&= b_{2j}(P^6_{\ell+3} \cup P_5 \cup P_1) + b_{2j-2}(P^6_{\ell+2} \cup P_4 \cup P_1) + b_{2j-4}(P^6_{\ell+2} \cup P_3)
\end{aligned}
$$

$$
\begin{aligned}
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_3\cup P_1)\\
&\quad +b_{2j-6}(P^6_{\ell}\cup P_3)\\
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_3\cup P_1)\\
&\quad +b_{2j-6}(P^6_{\ell}\cup P_2\cup P_1)+b_{2j-8}(P^6_{\ell}\cup P_1)\\
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_3\cup P_1)\\
&\quad +b_{2j-6}(P^6_{\ell}\cup P_2\cup P_1)+b_{2j-8}(P^6_{\ell-1}\cup P_1\cup P_1)+b_{2j-10}(P^6_{\ell-2}\cup P_1)
\end{aligned}
$$

and

$$
b_{2j-2}(P^6_{\ell+4}\cup P_2\cup P_1)=b_{2j-2}(P^6_{\ell+3}\cup P_1\cup P_2\cup P_1)+b_{2j-4}(P^6_{\ell+2}\cup P_2\cup P_1)
$$

Similarly, we have

$$
b_{2j}(P^6_{\ell+3}\cup C_6)=b_{2j}(P^6_{\ell+3}\cup P_6)+b_{2j-2}(P^6_{\ell+3}\cup P_4)+2b_{2j-6}(P^6_{\ell+3})
$$

where

$$
\begin{aligned}
b_{2j}(P^6_{\ell+3}\cup P_6) &= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+3}\cup P_4)\\
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_4)\\
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_3\cup P_1)\\
&\quad +b_{2j-6}(P^6_{\ell+1}\cup P_2)\\
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_3\cup P_1)\\
&\quad +b_{2j-6}(P^6_{\ell}\cup P_2\cup P_1)+b_{2j-8}(P^6_{\ell-1}\cup P_2)\\
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_3\cup P_1)\\
&\quad +b_{2j-6}(P^6_{\ell}\cup P_2\cup P_1)+b_{2j-8}(P^6_{\ell-1}\cup P_1\cup P_1)+b_{2j-10}(P^6_{\ell-1})\\
&= b_{2j}(P^6_{\ell+3}\cup P_5\cup P_1)+b_{2j-2}(P^6_{\ell+2}\cup P_4\cup P_1)+b_{2j-4}(P^6_{\ell+1}\cup P_3\cup P_1)\\
&\quad +b_{2j-6}(P^6_{\ell}\cup P_2\cup P_1)+b_{2j-8}(P^6_{\ell-1}\cup P_1\cup P_1)+b_{2j-10}(P^6_{\ell-2}\cup P_1)\\
&\quad +b_{2j-12}(P^6_{\ell-3})
\end{aligned}
$$

and

$$
b_{2j-2}(P^6_{\ell+3}\cup P_4)=b_{2j-2}(P^6_{\ell+3}\cup P_3\cup P_1)+b_{2j-4}(P^6_{\ell+3}\cup P_2)
$$

Since $b_{2r}(P^6_{\ell+3})=b_{2r}(P^6_{\ell+2}\cup P_1)+b_{2r-2}(P^6_{\ell+1})$, it follows that $P^6_{\ell+2}\cup P_1\preceq P^6_{\ell+3}$ and hence $P^6_{\ell+4}\cup P^4_5\prec P^6_{\ell+3}\cup C_6$ by Lemma 2.3. So $H_1\prec H_2$. The proof is now complete. ∎

The following proposition is immediate by Lemmas 3.3, 3.4 and 3.5.

Proposition 3.6 *For any graph $H_1\in\mathcal{H}_{II}(n;a,4,k;\ell_1,3,\ell_3)$ where $\ell_1\geq 3$, $\ell_3\geq 3$, $a+\ell_1\geq 8$ and $k+\ell_3\geq 14$, there exists a graph $H_2\in\mathcal{H}_{II}(n;6,6,6;2,2,\ell)=P^{6,6,6}_n$ such that $H_1\prec H_2$.*

3.3 For (ii) of the graph class $\mathcal{H}_2^*$

Proposition 3.7 *For any graph $H_1 \in \mathcal{H}_{II}(n; a, b, k; 3, 3, 3)$ where $a \geq k \geq b \geq 8$, $a \equiv 2 \ (mod\ 4)$ and $k \equiv 2 \ (mod\ 4)$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; a, b, k; 2, \ell_2, \ell_3)$ such that $H_1 \prec H_2$.*

Proof. Fix parameter n. For any $H_1 \in \mathcal{H}_{II}(n; a, b, k; 3, 3, 3)$, we choose a graph $H_2 \in \mathcal{H}_{II}(n; a, b, k; 2, 3, 4)$ (see Figure 8). It suffices to show that $H_1 \prec H_2$. From Lemma 2.2, we

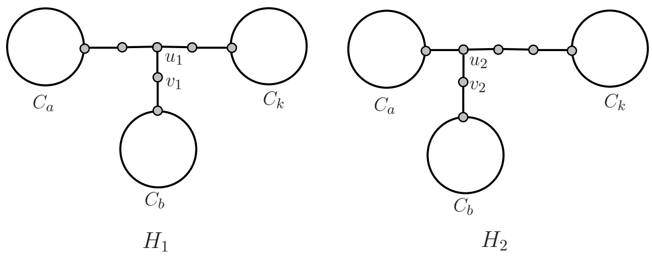


Figure 8: Graphs for Proposition 3.7.

have

$$\begin{aligned}
b_{2i}(H_1) &= b_{2i}(H_1 - u_1v_1) + b_{2i-2}(H_1 - u_1 - v_1) \\
&= b_{2i}(P^{a,k}_{a+k+3} \cup P^b_{b+1}) + b_{2i-2}(P^a_{a+1} \cup P^k_{k+1} \cup C_b) \\
b_{2i}(H_2) &= b_{2i}(H_2 - u_2v_2) + b_{2i-2}(H_2 - u_2 - v_2) \\
&= b_{2i}(P^{a,k}_{a+k+3} \cup P^b_{b+1}) + b_{2i-2}(C_a \cup P^k_{k+2} \cup C_b)
\end{aligned}$$

Applying Lemma 2.3, we only need to show that $P^a_{a+1} \cup P^k_{k+1} \prec C_a \cup P^k_{k+2}$.

From Lemma 2.2, we have

$$\begin{aligned}
b_{2j}(P^a_{a+1} \cup P^k_{k+1}) &= b_{2j}(C_a \cup P^k_{k+1} \cup P_1) + b_{2j-2}(P_{a-1} \cup P^k_{k+1}) \\
&= b_{2j}(C_a \cup P^k_{k+1} \cup P_1) + b_{2j-2}(P_{a-1} \cup C_k \cup P_1) + b_{2j-4}(P_{a-1} \cup P_{k-1}) \\
&= b_{2j}(C_a \cup P^k_{k+1} \cup P_1) + b_{2j-2}(P_{a-1} \cup C_k \cup P_1) \\
&\quad + b_{2j-4}(P_{a-2} \cup P_{k-1} \cup P_1) + b_{2j-6}(P_{a-3} \cup P_{k-1}) \\
b_{2j}(C_a \cup P^k_{k+2}) &= b_{2j}(C_a \cup P^k_{k+1} \cup P_1) + b_{2j-2}(C_a \cup C_k) \\
&= b_{2j}(C_a \cup P^k_{k+1} \cup P_1) + b_{2j-2}(P_a \cup C_k) + b_{2j-4}(P_{a-2} \cup C_k) \\
&\quad + 2(-1)^{1+\frac{a}{2}} b_{2j-2-a}(C_k) \\
&= b_{2j}(C_a \cup P^k_{k+1} \cup P_1) + b_{2j-2}(P_a \cup C_k) + b_{2j-4}(P_{a-2} \cup P_k) \\
&\quad + b_{2j-6}(P_{a-2} \cup P_{k-2}) + 2(-1)^{1+\frac{k}{2}} b_{2j-4-k}(P_{a-2} + 2(-1)^{1+\frac{a}{2}} b_{2j-2-a}(C_k)
\end{aligned}$$

Since $a \equiv 2 \ (mod\ 4)$ and $k \equiv 2 \ (mod\ 4)$, it follows that $2(-1)^{1+\frac{k}{2}} b_{2j-4-k}(P_{a-2}) \geq 0$ and $2(-1)^{1+\frac{a}{2}} b_{2j-2-a}(C_k) \geq 0$. Furthermore, $P_{a-3} \cup P_{k-1} \prec P_{a-2} \cup P_{k-2}$ since both a and k are even. One can easily see that $P^a_{a+1} \cup P^k_{k+1} \prec C_a \cup P^k_{k+2}$. Furthermore, we have $H_1 \prec H_2$. The proof is now complete. ∎

Remark 2. From the above proposition, for any graph $H \in \mathcal{H}_{II}(n; a, b, k; 3, 3, 3)$ where $a \geq k \geq b \geq 8$ and $a \equiv 2 \ (mod\ 4)$ and $k \equiv 2 \ (mod\ 4)$, H can not posses the maximal energy in $\mathcal{G}(n; a, b, k)$. So the remaining case is $a \geq k \geq b \geq 8$, and $a \equiv 0 \ (mod\ 4)$ or $k \equiv 0 \ (mod\ 4)$, which is stated as (ii) of the graph class $\mathcal{H}^{**}_2$ in Theorem 1.3.

3.4 For $(i), (iv)$ of the graph class $\mathcal{H}^*_2$ and (iii) of the graph class $\mathcal{H}^*_1$

In this section, we mainly discuss $(i), (iv)$ of the graph class $\mathcal{H}^*_2$, and the graph class (iii) of $\mathcal{H}^*_1$ is discussed in Remark 4.

Lemma 3.8 *For any graph $H_1 \in \mathcal{H}_{II}(n; a, b, k; 2, \ell_2, \ell_3)$ where $a \geq 8$, $\ell_2, \ell_3 \geq 3$, $b + \ell_2 \geq 8$ and $k + \ell_3 \geq 14$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; a, 6, 6; 2, \ell'_2, \ell'_3)$ such that $H_1 \preceq H_2$.*

Proof. Fix parameter n. For any graph $H_1 \in \mathcal{H}_{II}(n; a, b, k; 2, \ell_2, \ell_3)$ where $\ell_2, \ell_3 \geq 3$, $b + \ell_2 \geq 8$ and $k + \ell_3 \geq 14$, we choose a graph $H_2 \in \mathcal{H}_{II}(n; a, 6, 6; 2, \ell'_2, \ell'_3)$ such that $\ell'_2 = \ell_2 + b - 6$ and $\ell'_3 = \ell_3 + k - 6$ (see Figure 9). Clearly, $\ell'_3 \geq 8$. It suffices to show that $H_1 \preceq H_2$.

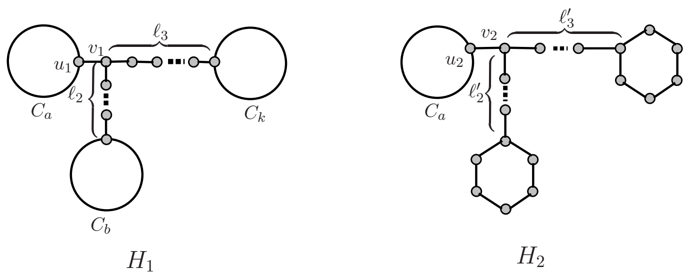


Figure 9: Graphs for Lemma 3.8

From Lemma 2.2, we have

$$\begin{aligned} b_{2i}(H_1) &= b_{2i}(H_1 - u_1v_1) + b_{2i-2}(H_1 - u_1 - v_1) \\ &= b_{2i}(P^{b,k}_{n-a} \cup C_a) + b_{2i-2}(P_{a-1} \cup P^b_{b+\ell_2-2} \cup P^k_{k+\ell_3-2}) \\ b_{2i}(H_2) &= b_{2i}(H_2 - u_2v_2) + b_{2i-2}(H_2 - u_2 - v_2) \\ &= b_{2i}(P^{6,6}_{n-a} \cup C_a) + b_{2i-2}(P_{a-1} \cup P^6_{\ell'_2+4} \cup P^6_{\ell'_3+4}) \end{aligned}$$

Because $\ell_2' = \ell_2+b-6$ and $\ell_3' = \ell_3+k-6$, we have $\ell_2'+4 = \ell_2+b-2$ and $\ell_3'+4 = \ell_3+k-2$. Therefore, $P^b_{\ell_2+b-2} \preceq P^6_{\ell_2'+4}$, $P^k_{\ell_2+k-2} \preceq P^6_{\ell_3'+4}$ and $P^{b,k}_{n-a} \preceq P^{6,6}_{n-a}$. Lemma 2.3 yields $H_1 \preceq H_2$, as desired. ∎

Lemma 3.9 *For any graph $H_1 \in \mathcal{H}_{II}(n; a, 6, 6; 2, \ell_2, \ell_3)$ where $\ell_3 \geq 8$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; a, 6, 6; 2, 2, \ell)$ such that $H_1 \prec H_2$.*

Proof. Fix parameter n. For any graph $H_1 \in \mathcal{H}_{II}(n; a, 6, 6; 2, \ell_2, \ell_3)$ where $\ell_3 \geq 8$, we choose a graph $H_2 \in \mathcal{H}_{II}(n; a, 6, 6; 2, 2, \ell)$ such that $\ell = \ell_2 + \ell_3 - 2$ (see Figure 10). Since $\ell_2 \geq 2$ and $\ell_3 \geq 8$, it follows that $\ell \geq 8$. It suffices to show that $H_1 \prec H_2$. From Lemma 2.2, we have

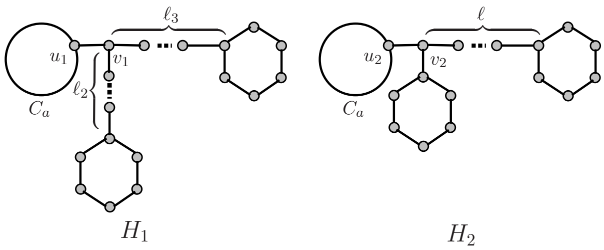


Figure 10: Graphs for Lemma 3.9

$$
\begin{aligned}
b_{2i}(H_1) &= b_{2i}(H_1 - u_1v_1) + b_{2i-2}(H_1 - u_1 - v_1) \\
&= b_{2i}(P^{6,6}_{n-a} \cup C_a) + b_{2i-2}(P_{a-1} \cup P^6_{\ell_2+4} \cup P^6_{\ell_3+4}) \\
b_{2i}(H_2) &= b_{2i}(H_2 - u_2v_2) + b_{2i-2}(H_2 - u_2 - v_2) \\
&= b_{2i}(P^{6,6}_{n-a} \cup C_a) + b_{2i-2}(P_{a-1} \cup P^6_{\ell+4} \cup C_6)
\end{aligned}
$$

Similarly to the proof of Lemma 3.4, we can obtain $P^6_{\ell_2+4} \cup P^6_{\ell_3+4} \prec P^6_{\ell+4} \cup C_6$. From Lemma 2.3, we have $H_1 \prec H_2$, as desired. ∎

Proposition 3.10 *For any graph $H_1 \in \mathcal{H}_{II}(n; a, b, k; 2, \ell_2, \ell_3)$ where $a \geq 8$, $\ell_2 \geq 3$, $\ell_3 \geq 3$, $b + \ell_2 \geq 8$ and $k + \ell_3 \geq 14$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; a, 6, 6; 2, 2, \ell)$ such that $H_1 \prec H_2$.*

Similarly to the proof of Proposition 3.10, we can derive the following result.

Proposition 3.11 *For any graph $H_1 \in \mathcal{H}_{II}(n; a, 4, k; \ell_1, 2, \ell_3)$ where $\ell_1 \geq 3$, $\ell_3 \geq 3$, $a + \ell_1 \geq 8$, $k + \ell_3 \geq 14$, there exists a graph $H_2 \in \mathcal{H}_{II}(n; 6, 4, 6; 2, 2, \ell)$ such that $H_1 \prec H_2$.*

Remark 3. From the above propositions, for (i) of the graph class $\mathcal{H}_2^*$, the remaining graph classes under consideration are $\mathcal{H}_{II}(n; a, b, k; 2, \ell_2, \ell_3) \cup \mathcal{H}_{II}(n; a, 6, 6; 2, 2, \ell)$, where $a \geq 8$, $\ell \geq$

8, and $\ell_2 = 2$ or $\ell_3 = 2$ or $6 \leq b+\ell_2 \leq 7$ or $6 \leq k+\ell_3 \leq 13$; for (iv) of the graph class $\mathcal{H}_2^*$, the remaining graph classes under consideration are $\mathcal{H}_{II}(n; a, 4, k; \ell_1, 2, \ell_3) \cup \mathcal{H}_{II}(n; 6, 4, 6; 2, 2, \ell)$, where $\ell \geq 8$, and $\ell_1 = 2$ or $\ell_3 = 2$ or $6 \leq a + \ell_1 \leq 7$ or $6 \leq k + \ell_3 \leq 13$.

Remark 4. For any $H \in \mathcal{H}_I(n; 4, b, k; \ell_1, \ell_2; 2)$ where $b \geq 6$, $k \geq 6$, $2 \leq \ell_1 \leq 3$ and $2 \leq \ell_2 \leq 3$, one can see that $H \in \mathcal{H}_I(n; a, b, 4; \ell_1, \ell_2; 2)$ where $2 \leq \ell_2 \leq 3$. This observation suggests that the graph class (iii) of $\mathcal{H}_1^*$ is a subset of the graph class (iv) of $\mathcal{H}_1^*$, thus omitted and deleted in Theorem 1.3.

References

[1] E. O. D. Andriantiana, Unicyclic bipartite graphs with maximum energy, *MATCH Commun. Math. Comput. Chem.* **66**(2011), 913–926.

[2] E. O. D. Andriantiana, S. Wagner, Unicyclic graphs with large energy, *Linear Algebra Appl.* **435**(2011), 1399–1414.

[3] M. Aouchiche, G. Caporossi, P. Hansen, Open problems on graph eigenvalues studied with AutoGraphiX, *EURO J. Comput. Optim.* **1**(2013), 181–199.

[4] J. A. Bondy, U. S. R. Murty, *Graph Theory*, GTM 244, Springer, 2008.

[5] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39**(1999), 984–996.

[6] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs − Theory and Application*, Academic Press, New York, 1980.

[7] B. Furtula, S. Radenković, I. Gutman, Bicyclic molecular graphs with the greatest energy, *J. Serb. Chem. Soc.* **73**(2008), 431–433.

[8] I. Gutman, Acylclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta.* **45**(1977), 79–87.

[9] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer, Berlin, (2001), 196–211.

[10] I. Gutman, X. Li, J. Zhang, Graph Eenergy, in: M. Dehmer, F.Emmert-Streb(Eds.), *Analysis of Complex Networks: From Biology to Linguistics*, Wiley-VCH Verlag, Weinheim. (2009), 145–174.

[11] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.

[12] I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: a computer experiment, *J. Chem. Inf. Sci.* **41**(2001), 1002–1005.

[13] Y. Hou, Unicyclic graphs with minimal energy, *J. Math. Chem.* **29**(2001), 163–168.

[14] Y. Hou, Bicyclic graphs with minimal energy, *Lin. Multilin. Algebra.* **49**(2002), 347–354.

[15] Y. Hou, I. Gutman, C. Woo, Unicyclic graphs with maximal energy, *Linear Algebra Appl.* **356**(2002), 27–36.

[16] B. Huo, J. Ji, X. Li, Note on unicyclic graphs with given number of pendant vertices and minimal energy, *Linear Algebra Appl.* **433**(2010), 1381–1387.

[17] B. Huo, J. Ji, X. Li, Solutions to unsolved problems on the minimal eneries of two classes of graphs, *MATCH Commun. Math. Comput. Chem.* **66**(2011), 943–958.

[18] B. Huo, J. Ji, X. Li, Y. Shi, Complete solution to a conjecture on the fourth maximal energy tree, *MATCH Commun. Math. Comput. Chem.* **66**(2011), 903–912.

[19] B. Huo, S. Ji, X. Li, Y. Shi, Solution to a conjecture on the maximal energy of bipartite bicyclic graphs, *Linear Algebra Appl.* **435**(2011), 804–810.

[20] B. Huo, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of unicyclic bipartite graphs, *Linear Algebra Appl.* **434**(2011), 1370–1377.

[21] B. Huo, X. Li, Y. Shi, Complete solution to a conjecture on the maximal energy of uncicyclic graphs, *Europ. J. Combin.* **32**(2011), 662–673.

[22] B. Huo, X. Li, Y. Shi, L. Wang, Determining the conjugated trees with the third through the sixth minimal energies, *MATCH Commun. Math. Comput. Chem.* **65**(2011), 521–532.

[23] F. Li, B. Zhou, Minimal energy of bipartire unicyclic graphs of a given bipartition, *MATCH Commun. Math. Comput. Chem.* **54** (2005), 379–388.

[24] S. Li, X. Li, On tetracyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem.* **60**(2008), 395–414.

[25] S. Li, N. Li, On minimal energies of acyclic conjugated molecules, *MATCH Commun. Math. Comput. Chem.* **61**(2009), 341–349.

[26] S. Li, X. Li, On tricyclic graphs of a given diameter with minimal energy, *Linear Algebra Appl.* **430**(2009), 370–385.

[27] S. Li, X. Li, Z. Zhou, On tricyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem.* **59**(2008), 397–419.

[28] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.

[29] X. Li, Y. Shi, M. Wei, J. Li, On a conjecture about tricyclic graphs with maximal energy, *MATCH Commun. Math. Comput. Chem.* **72(1)**(2014), 183–214.

[30] X. Li, J. Zhang, On bicyclic graphs with maximal energy, *Linear Algebra Appl.* **427**(2007), 87–98.

[31] X. Li, J. Zhang, L. Wang, On bipartite graphs with minimal energy, *Discr. Appl. Math.* **157**(2009), 869–873.

[32] S. Wagner, Energy bounds for graphs with fixed cyclomatic number, *MATCH Commun. Math. Comput. Chem.* **68**(2012), 661–674.

[33] F. Zhang, H. Li, On acyclic conjugated molecules with minimal energy, *Discr. Appl. Math.* **92**(1999), 71–84.